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L X-ray satellites of silicon

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Abstract : The average energies of *L* X-ray satellites of silicon with one to two spectator vacancies in the M_1 or $M_{2,3}$ subshells are calculated in this work using a judicious mixture of sudden and adiabatic models. The total average energies of the various defect-electron configurations needed in the evaluation of the transition energies have been calculated in the *LS* coupling scheme using relativistic Dirac-Fock values of direct and exchange integrals.

Keywords : X-ray spectra, satellite lines, spectator vacancy, defect-electron configurations

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1. Introduction

It is well known that X-ray diagram lines are often accompanied on both high and low frequency sides by several weak lines called satellite lines. The high energy satellites are generally attributed to multiple ionisation of atoms in different shells. During natural processes like *K*-shell shake off following β decay [1] and artificial processes like photon, electron or ion-atom interactions [2], multiple vacancies are created in the target atoms. Radiative decay of the inner shell vacancies of these ionised atoms yields a series of satellite and hypersatellite lines on the high energy side of the diagram lines. The spectral features of the emitted radiations are of importance in the study of astrophysical and laboratory induced fusion plasmas [3], soft X-ray lasers [4], chemical analysis of materials [5] etc.

The *L* X-ray satellites are due to the transitions of electrons in the *M,N* etc. shells to the *L*-shell in the presence of spectator vacancies in the *M,N* etc. shells. Though theoretical calculations on the energies of *L* X-ray satellites arising from electric dipole and quadrupole transitions in the presence of single or multiple spectator holes in the *M* shell exist for heavy elements [6,7], no such systematic calculations seem to have been carried out for light elements. Hence in the present work an attempt has been made to calculate the average energies of *L* X-ray satellites of silicon with one to two spectator holes in the M_1 or $M_{2,3}$ shells. The purpose of choosing silicon is that it has wide practical applications and is found as an impurity atom in astrophysical and laboratory plasmas. Moreover, being a light element, the *LS* coupling approximation used in this work is valid.

2. Procedure for calculation

The total average energies of an atom in various defect electron configurations are needed to calculate the energies of the satellite lines. The relativistic expression for the *LS* average energies of neutral and ionised atoms obtained from Slater's [8] non-relativistic expression is given by.

$$E_{av}^{R} = \underset{\text{(all)}}{I^{R}(nlj)} + \underset{\text{(pairs)}}{\text{interaction energies}} \tag{1}$$

where I^R(nlj) is the relativistic one-electron energy integral. The electrostatic energies are given in terms of direct F^K and exchange G^K integrals. The relativistic expressions for the one electron integrals and direct and exchange integrals are given by Larkins [9].

Two alternative approaches can be used to calculate the average energies of a particular configuration. In the sudden model, the total energies of ionised states are calculated using neutral atom wavefunctions. In the more realistic adiabatic model, complete relaxation of orbitals is taken into account and the energies of the different ionised state are computed separately by considering appropriate wavefunctions corresponding to these states. In this work, a judicious mixture of sudden and adiabatic models has been used. The average energies of different configurations have been calculated using sudden model. However, following Larkins [9], a correction term corresponding to the adiabatic relaxation of orbitals has also been taken into account.

The relativistic one-electron energies have been calculated using orbital exponents derived from neutral atom self consistent field wavefunctions [10]. The relativistic Dirac Fock values of direct and exchange integrals have been taken from the compilation of Aoyogi *et al* [11]. The average energies of the different configurations evaluated using eq. (1) are then corrected for relaxation effects. These values have been taken from the work of Larkins [12].

3. Results

Table 1 lists the energies of *L* X-ray satellites of silicon. In this table, the different defect electron configurations are indicated by the missing electrons in the initial and final states. Column 1 of this table corresponds to initial configuration and column 2 represents final configuration. Column 3 gives the energies of the various *L* X-ray satellites of silicon arising due to multiple ionisation. Column 4 reports the energy shifts ΔE of the different *L* X-ray satellite lines from their respective diagram lines. An average energy shift is obtained by summing the energy shifts of the various *L* X-ray satellites and dividing by the sum of the *M*-shell vacancies. This gives information about the number of *M*-shell vacancies in addition to the single vacancy in the *L*-shell present at the time of *L* X-ray emission. In this work, an average energy shift of 3.52 eV per *M*-shell spectator vacancy for $L_1^{-1} M^{-1} \rightarrow M^{-2}$ transitions is obtained. Similarly for $L_{2\,3}^{-1} M^{-1} \rightarrow M^{-2}$ transitions, the average shift per *M*- vacancy turns out to be 1.27 eV. It may be noted that the distinction

between M_1 and $M_{2,3}$ electrons has not been taken into account while calculating the average energy shifts.

Table 1. Energies of L X-ray satellites of silicon in eV.

initial configuration	final configuration	energies in eV	energy shifts in eV
$2s^{-1}$	$3p^{-1}$	145 7	
$2s^{-1}$ $3p^{-1}$	$3p^{-2}$	148.1	2.4
$2s^{-1}$ $3s^{-1}$	$3s^{-1}$ $3p^{-1}$	149.7	4.0
$2s^{-1}$ $3s^{-1}$ $3p^{-1}$	$3s^{-1}$ $3p^{-2}$	152.0	6.3
$2s^{-1}$ $3s^{-2}$	$3s^{-2}$ $3p^{-1}$	[illegible]	8 0
$2s^{-1}$ $3s^{-2}$ $3p^{-1}$	$3s^{-2}$ $3p^{-2}$	155.8	10.1
$2p^{-1}$	$3s^{-1}$	91 6	
$2p^{-1}$ $3p^{-1}$	$3s^{-1}$ $3p^{-1}$	92.8	1 2
$2p^{-1}$ $3s^{-1}$	$3s^{-2}$	93 1	1.5
$2p^{-1}$ $3s^{-1}$ $3p^{-1}$	$3s^{-2}$ $3p^{-1}$	93 5	2.0
$2p^{-1}$ $3p^{-2}$	$3s^{-1}$ $3p^{-2}$	94.1	2.5
$2p^{-1}$ $3s^{-1}$ $3p^{-2}$	$3s^{-2}$ $3p^{-2}$	95.8	4.2

4. Conclusion

Though considerable amount of experimental and theoretical study exits for the K X-ray satellites of silicon arising due to multiple spectator vacancy in the L-shell, similar work for the L X-ray satellites are not available. As such studies give valuable information on the different transient states of atoms ionised to different degrees, it is worthwhile to carryout a systematic experimental and theoretical study on the L X-ray satellites of different elements in the periodic table.

References

[1] Y Isozumi and A Shimizu 1971, *Phys. Rev* **C4** 522

[2] P Richard 1976 in *Atomic Innershell Processes* ed. B Crasemann (New York · Academic)

[3] M Bitter, K W Hill, M Zarnstorff, S Von Goeler, R Hulse, L Johnson, N R Sauthoff, M Tavernier, F Bely-Dubau, P Faucher, M Cornille and J Dubau 1985 *Phys Rev* **A32** 3011

[4] A Tanis, E M Berster, W G Graham, M Clark, S M Shafroth, B M Johnson, K W Jones and M Meron 1982 *Phys. Rev Lett.* **49** 1325

[5] S Raman 1983 in *Applied Atomic Collisions* ed Date Sheldon (New York Academic) Vol. 4

[6] F Parente, M H Chen, B Crasemann and H Mark 1981 *At. Data Nucl. Data Tables* **26** 383

[7] W Uchai, C W Nestor Jr, S Raman, and C R Vane 1986 *At. Data. Nucl. Data Tables* **34** 291

[8] J C Slater 1960 *Quantum Theory of Atomic Structure* (New York : MacGraw Hill) Vol. 1

[9] F Larkins 1976 *J. Phys.* **B9** 47

[10] E Clementi and D L Raimondi 1963 *J. Chem. Phys.* **38** 2686

[11] M Aoyagi, M H Chen, K N Huang, B Crasemann and H Mark 1976 *Relativistic Electrostatic Integrals* NASA TMX **73** 148

[12] F Larkins 1977 *At. Data Nucl. Data Tables* **20** 311